

Investigation of Surface and Bulk Half-metallic Character of Fe_3O_4 by Spin Resolved Photoemission

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The existence of a new class of magnetic materials displaying metallic character for one electron spin population and insulating character for the other was first postulated by DeGroot *et al* [1] in 1983 based on theoretical band structure calculations of the ferromagnetic Heusler alloy NiMnSb. Since then such half metallic materials, which by definition possess 100% electron polarization at the Fermi energy have attracted considerable theoretical, experimental, and technological interest as potential pure spin sources for use in spintronic devices [2], data storage applications, and magnetic sensors. In addition to Heusler alloys half metallic character has also been predicted to occur in a wide range of manganites [3], metallic oxides [4], and CMR systems [5]. However, such predictions have proven to be extremely difficult to confirm experimentally [6]. A major factor in this failure has proven to be significant experimental challenges in obtaining a clean stoichiometric surface with a magnetization that is truly representative of the bulk material and thus suitable for further study by magneto-optical or spectroscopic techniques.

In recent experiments at the ALS we have used spin resolved photoemission to study the role that surface reconstruction plays in the observed polarization of the half metallic candidate material magnetite, Fe_3O_4 . Magnetite has a structure that is relatively simple in comparison to most other candidate half metals and it can be grown epitaxially using conventional deposition techniques [7], making it one of the strongest candidates for spintronic applications. However previous spin resolved measurements have shown that the polarization at the Fermi edge is only ~40% [8] rather than the anticipated 100%.

By conducting spin resolved depth profile measurements and comparing the results to theoretical band structure calculations we have demonstrated that Fe_3O_4 exhibits a semiconducting non-magnetic surface re-construction which significantly reduces the observed polarization but that, in contrast, the underlying bulk material is in fact very strongly polarized. Indeed, once the effects of this surface reconstruction are taken into account by theoretical models of the polarization an excellent match is obtained between the experimental spin resolved spectra and simulated spectra generated from theoretical spin polarized band structure calculations [9] (fig. 1). Hence our results strongly support the notion that Fe_3O_4 is indeed a half-metallic material suitable for use in a new generation of spintronic devices.

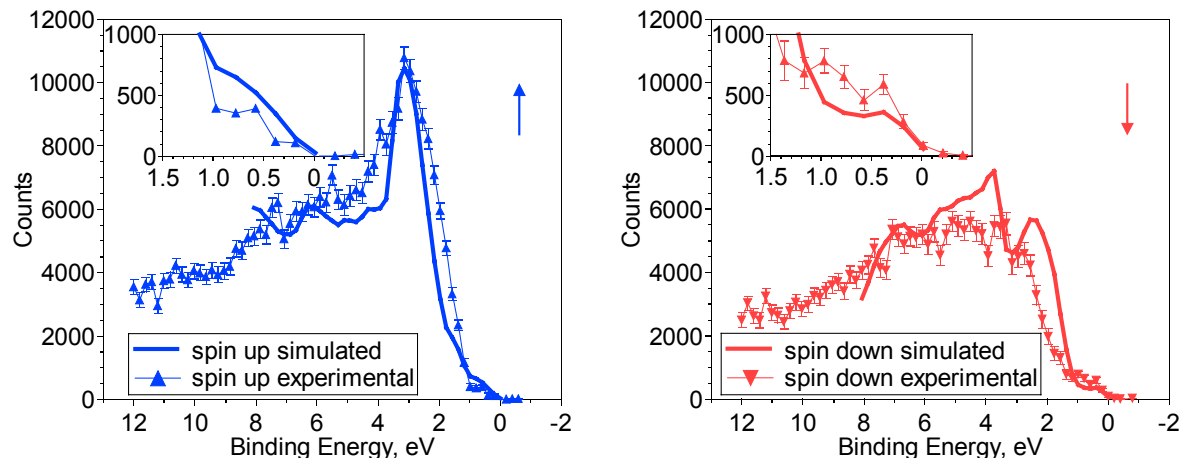


Figure 1

Comparison of experimental spin resolved Fe_3O_4 valence bands with equivalent simulated spectra derived from theoretical calculations that have been corrected to account for the presences of a nonmagnetic surface reconstruction

References

1. R. A. de Groot *et al.*, *Phys. Rev. Lett.* **50**, 2024 (1983).
2. S. A. Wolf, D. Treger, *IEEE Trans. Mag.* **36** 2748 (2000).
3. S. Jin *et al.*, *Science* **264**, 413 (1994).
4. Z Zhang, S. Satpathy, *Phys. Rev. B* **44**, 13319 (1991).
5. W. E. Pickett, D. J. Singh, *Phys. Rev. B* **53**, 1146 (1996).
6. K. P. Kamper *et al.*, *Phys. Rev. Lett.* **59** 2788 (1987).
7. S. A. Chambers, S. A. Joyce, *Surf. Sci.* **420**, 111 (1999).
8. S. F. Alvarado *et al.*, *Phys. Rev. Lett.* **34**, 319 (1975).
9. S.A. Morton *et al.*, *Submitted to Surface Science Letters*

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